Abstract Submitted
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A Novel Quasi-One-Dimensional Topological Insulator in Bismuth Iodide β-Bi_4I_4: Theoretical Prediction and Experimental Confirmation[1] OLEG V. YAZYEV, GABRIEL AUTÈS, EPFL, ANNA ISAEVA, TU Dresden, LUCA MORESCHINI, LBNL, JENS C. JOHANNSEN, ANDREA PISONI, EPFL, TAISIA G. FILATOVA, ALEXEY N. KUZNETSOV, MSU, LÁSZLÓ FORRÓ, EPFL, WOUTER VAN DEN BROEK, Ulm University, YEONGKWAN KIM, JONATHAN D. DENLINGER, ELI ROTENBERG, AARON BOSTWICK, LBNL, MARCO GRIONI, EPFL — A new strong Z_2 topological insulator is theoretically predicted and experimentally confirmed in the β-phase of quasi-one-dimensional bismuth iodide Bi_4I_4. According to our first-principles calculations the material is characterized by Z_2 invariants (1;110) making it the first representative of this topological class. Importantly, the electronic structure of β-Bi_4I_4 is in proximity with both the weak topological insulator phase (0;001) and the trivial phase (0;000), suggesting that a high degree of control over the topological electronic properties of this material can be achieved. Experimentally produced samples of this material appears to be practically defect-free, which results in a low concentration of intrinsic charge carriers. By using angle-resolved photoemission spectroscopy (ARPES) on the (001) surface we confirm the theoretical predictions of a highly anisotropic band structure with a small band gap hosting topological surface states centered at the $\bar{M}$ point, at the boundary of the surface Brillouin zone.

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